

COSMOquick 1.3 Release Notes (10/2014)

COSMOquick is a powerful toolbox without need for costly quantum chemistry calculation. It provides accurate solubility calculations, QSPR-predictions and descriptors, cocrystal screening, input files for COSMOtherm and much more.

New features of version 1.3:

- Solute backfitting: sigma-profile creation for an unknown or undetermined compound by using only its reference solubilities in different solvents
- QSPR builder: Use COSMOquick variables to generate and deploy meaningful quantitative structure property relationship (QSPR) models; includes automatic variable selection and cross-validation
- Determination of Hansen solubility parameters via solubility calculations
- Extended .cosmo file database for better sigma profile generation

Other improvements: new look&feel, improved handling of stereoisomers, enhanced 3D structure generation, additional plotting functionality, new descriptors & QSPR models

Additionally, the following tasks can be carried out with COSMOquick::

- Accurate solubility prediction using multiple reference solvents
- QSPR predictions using multi-linear regression or random forest based models
- Cocrystal screening, i.e. fast calculations of excess enthalpies
- Sorption of small molecules in polymers or solvents
- ADME property calculations, i.e. different partition coefficients and water solubility
- Approximate σ -profiles for use with COSMOtherm

Furthermore a few other useful features are available and suitable for an easy processing of large amount of data (resolution of SMILES from names or CAS numbers, 2D structure editor, SMARTS handling).

Fragmentation Approach: COSMOquick uses a unique approach for the generation of σ -profiles (Hornig, M. & Klamt, A. *J Chem Inf Model*, **2005**, 45, 1169.). The basic idea is the composition of the σ -profile of a new molecule from existing molecules that have already been pre-calculated. Thus no quantum chemistry calculation is needed.

Limitations: Currently the following limitations are inherent to the fragmentation approach used to generate the σ -profile:

- σ -profile are only approximate (except for an exact match in the database)
- classic quantum chemistry may still be needed for some ions and for very rare functional groups
- no conformer treatment possible
- BP-SVP parameterization only

System requirements: COSMOquick is available for operating systems Windows, Linux and MacOS. Recommended Hardware for the CFDB (COSMOfrag-Database): 2.5 GB disk space. Additional hard disc space for temporary data is needed.

You may also visit our homepage: <http://www.cosmologic.de/products/cosmoquick.html>